Light Scattering by Marine Particles: Modeling with Non-spherical Shapes

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LONG-TERM GOALS

The long-term scientific goal of my research is to better understand the distribution of phytoplankton in the world's oceans through remote sensing their influence on the optical properties of the water. An associated goal is the understanding of the absorption and backscattering properties of marine particles in terms of the distributions of their size, shape, and composition.

OBJECTIVES

The inherent optical properties (IOPs) of marine particles are most-often modeled as homogeneous spheres using Mie Theory. Although this approach has been fruitful, the next logical step in modeling marine particles is to abandon the normally-employed spherical approximation and use more realistic approximations to their shape. The advent of computer codes capable of handling more complex shapes, and the increased computational speeds now available, suggest that particle modeling employing simple non-spherical shapes, e.g., disks, rods, etc., could become routine. For example, Gordon and Du (2001) used a two-disk model to try to reproduce the backscattering by coccoliths detached from *E. huxleyi*; however, they found that, while the resulting spectral variation of the backscattering cross section agreed with experiment, its magnitude was low by a factor of 2-3. Such simple shapes are still at best poor approximations to real particles, as real particles display significant inhomogeneity.

It is often assumed that inhomogeneous particles can be replaced by homogeneous particles along with employing an “effective” refractive index; however, my study of thin disks showed the importance of periodic angular fine scale structure and demonstrated that if the inhomogeneities are too large, the effective refractive index assumption is invalid and the backscattering increases significantly over that expected based on the effective index hypothesis. Thus, in attempting to model with shapes other than spherical, we are still left with the question of the relative importance of gross morphology and fine structure. To apply, with confidence, scattering computations based on simple particle shapes to explain or interpret observed particle backscattering, it is important to understand how deviations from simple shapes or how non-homogeneity of composition, affect the scattering and absorption of light. The objective of this study is to continue the development of such an understanding.

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APPROACH

I use detached coccoliths from the coccolithophorid *E. huxleyi* (Figure 1) as a case study for applying non-spherical shapes to the computation of backscattering. This particle was chosen because (1) its composition is known and homogeneous (refractive index $m \approx 1.20$), (2) its gross shape is known (it resembles a disk or two parallel disks), (3) its optical properties are known, and (4) it has a complex, quasi-periodic internal structure on a sub-visible-wavelength scale. Gordon (2006) focused on the quasi-periodic structure of the top disk (in Figure 1) and on the influence of the curvature of the lower plate. (The influence of the curvature was found to be small and will not be discussed here.)

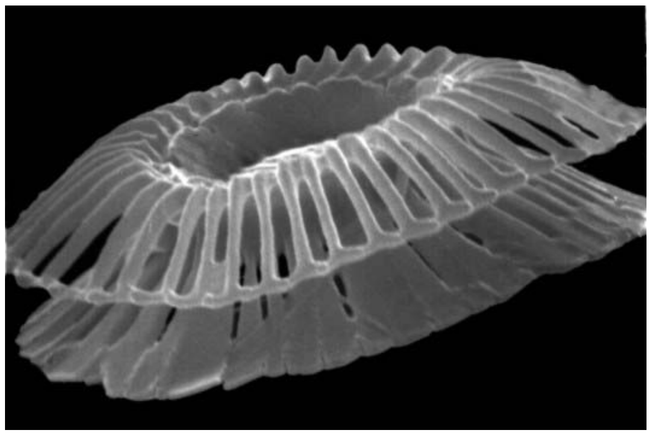
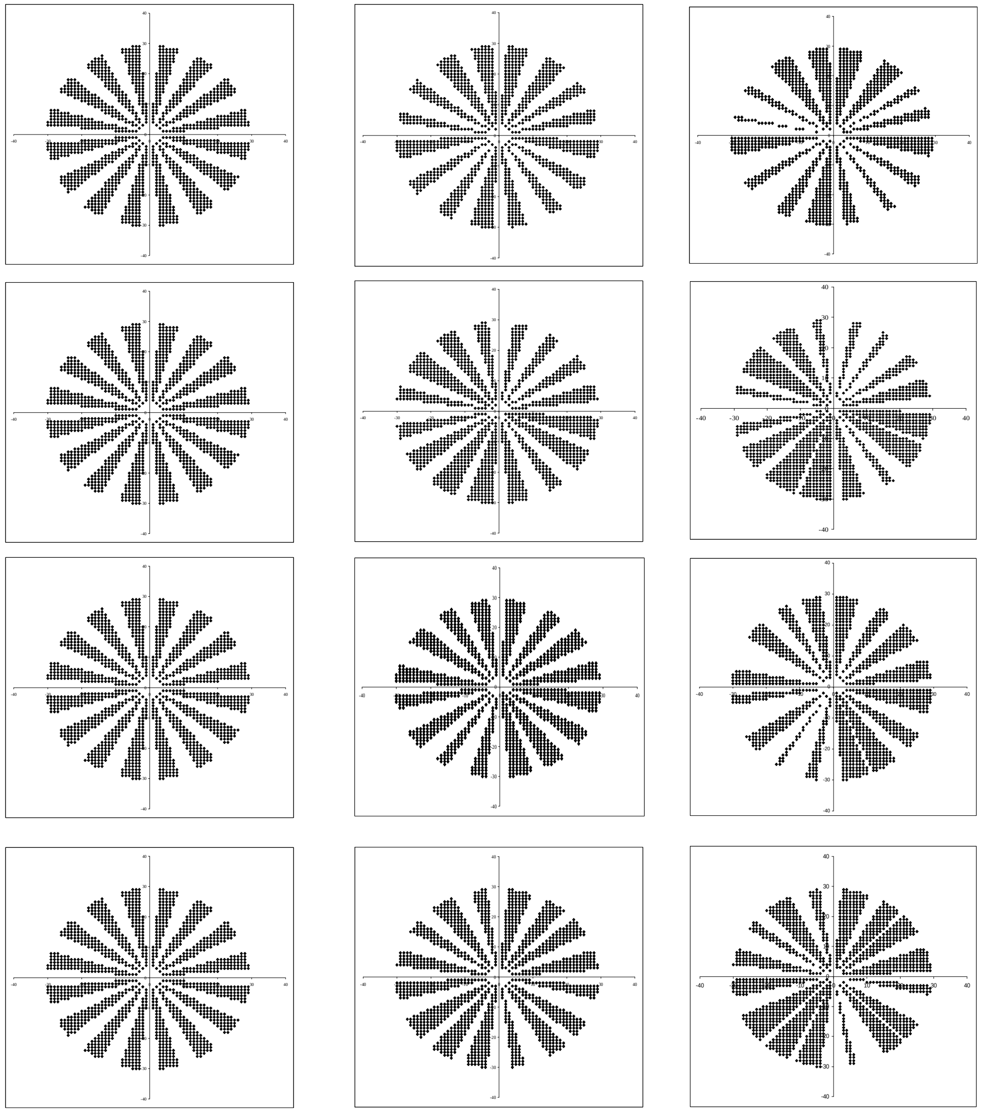


Figure 1: SEM image of coccolith a detached from E. huxleyi showing a structure grossly resembling two parallel disk-like plates. The upper plate resembles a wheel with spokes. The spoke separation is 50 to 150 nm.

I use the term "gross morphology" to indicate a smooth homogeneous particle having approximately the same overall shape as the particle in question (e.g., a single disk or two parallel disks as a model for a detached coccolith). I use "fine-scale structure" to indicate deviations from the gross morphology (e.g., the coccolith's periodic radial structures resembling the openings between the spokes of a wagon wheel). My goal is to understand how the fine-scale structure can induce deviations in the backscattering characteristic of a given gross morphology. Since the physical example of interest is a coccolith, I limit the examination to particles with the gross morphology of a disk.

To investigate the influence of periodic fine structure in a disk-like object on backscattering, I started with a homogeneous disk and removed sectors. Specifically, the disk was divided into equal angle sectors of angle $\Delta\alpha$, and alternate sectors were removed. The angle $\Delta\alpha$ was given by $\Delta\alpha = 2\pi/2^n$, where n is an integer. I refer to these objects as "pinwheels." (See Figure 2, $\varepsilon = 0$ column, for an example of a pinwheel with $n = 5$.) If we let s be the arc length of the open (or closed) regions at the perimeter of the pinwheel, then $s = D\Delta\alpha/2$, where D is the diameter



$\varepsilon = 0$ $\varepsilon = 0.5$ $\varepsilon = 1.0$

Figure 2: The individual rows provide four realizations of the aperiodic pinwheels for n = 5 and various values of ε. Periodic pinwheels are shown in the first column. For the aperiodic pinwheels, the individual vanes have random angular extent. The departure from the periodic pinwheel increases with increasing ε.

of the disk (1.5 μm). The values of *s* for the various cases that I examined were such that at a wavelength (λ) of 400 nm in vacuum (300 nm in water), as *n* progresses from 4 to 7, *s* takes on the values λ, $\lambda/2$, $\lambda/4$, and $\lambda/8$ in water. One of the main goals of my study was to determine if a relationship exists between *s* and λ where the periodic structure becomes important (or unimportant) to the backscattering. I computed the backscattering cross section σ_b of pinwheels using the discrete-dipole approximation (Draine,1988; Draine and Flatau, 1994). The computations showed that their backscattering cross section was nearly identical to that of a homogeneous disk of similar size (but with m reduced from 1.20 to $m_{eff} = 1.10$) as long as $s/\lambda_{Water} < 0.25$. Pinwheels satisfying this criterion also scattered in the same manner as disks having half of the mass removed from random locations within the disk. Thus, when $s/\lambda_{Water} < 0.25$, there is essentially no difference in backscattering between the periodic structure and a structure of small random voids (in disk-like particles) with the same total mass. In this regime the backscattering is totally governed by the particle's gross morphology and effective index (m_{eff}). For $s/\lambda_{Water} > 0.25$ departures from a homogeneous disk are observed and manifest as a significant increase (many times) in backscattering: the fine-scale structure is as important as the gross morphology in this regime.

In the present work I continue exploration of the backscattering by objects possessing small-scale structure. I focus on (1) extending the sectorized disk studies (Gordon 2006) to larger t/λ_{Water} in order to understand how large σ_b will eventually become when $s/\lambda_{Water} > 0.25$, (2) extending the computations to sectorized disks with *aperiodic* structure to try to understand the influence of non-uniform spacing of the spokes in the upper plate of the coccolith (Figure 1) and (3) building a fine-scale model of a detached coccolith for computation of the coccolith-specific σ_b.

WORK COMPLETED

I formed aperiodic pinwheels through a perturbation of the purely periodic pinwheel effected in the following manner. First, as before, the disk is divided into purely periodic sectors, the angular boundaries of which are designated by the 2^n angles α_P. The individual boundary angles are then perturbed to α_I according to

$$\alpha_I = \alpha_P + \varepsilon \frac{2\pi}{2^n}\rho ,$$

where $0 \le \varepsilon \le 1$ is a constant and $-1/2 \le \rho \le 1/2$ is a random number with a uniform probability density. Then, the material of the disk is removed from ever other sector, yielding a pinwheel with a quasi-periodic structure. Four realizations (each based on a difference sequence of pseudorandom numbers) of such pinwheels for $n = 5$ are provided in Figure 2 for $\varepsilon = 0.5$ and 1.0 in the second and third columns, respectively. Defining σ_I to be the standard deviation in the angle α_I, we find $\sigma_I = 12^{-½}\varepsilon\,\Delta\alpha \approx 0.3\varepsilon\,\Delta\alpha$, where $\Delta\alpha = 2\pi/2^n$. Likewise defining $\sigma_{\Delta\alpha}$ to be the standard deviation of the removed (or occupied) sector angles, $\sigma_{\Delta\alpha} = 6^{-½}\varepsilon\,\Delta\alpha \approx 0.4\varepsilon\,\Delta\alpha$. Thus, for $\varepsilon = 0.5$ and 1.0, the relative standard deviation in angle of the removed (or occupied) sectors is 20 and 40%, respectively. I examined three aperiodic pinwheels. The first has a diameter (D) of 1.50 μm, a thickness (t) of 0.15 μm, and $n = 5$ (Figure 2), the second has $D = 2.75$ μm, $t = 0.05$ μm, and $n = 6$, and the third has $D = 1.50$ μm, $t = 0.05$ μm, and $n = 5$. The larger-diameter disk is similar in size to the distal shield (top plate) of individual *E. huxleyi* coccoliths (Figure 1).

The individual realizations are labeled by the one minus the position in a string of pseudorandom numbers where the sampling for ρ begins. Thus, for realization 0000 the sampling begins with the first number, for realization 1000 it begins with the 1001th number, etc. This method of creating aperiodic pinwheels does not yield structures with the same volume (mass) as the associated periodic pinwheel. The variation of the volume for a given ε can be as much as 25% for the smaller ($D = 1.5$ μm, $n = 5$) and 7% for the larger ($D = 2.75$ μm, $n = 6$) pinwheels. The reduction in dispersion from the smaller to the larger is due to the increase in n, which doubles the number of sectors, increasing the probability that the individual realizations have a volume closer to the mean.

The scattering computations were carried out using the discrete-dipole approximation (DDA) operating on a 40 CPU cluster. The accuracy of the DDA for randomly oriented particles is governed by two issues: (1) employing a sufficient number of dipoles to solve the electromagnetic scattering problem for a given orientation; and (2) employing a sufficient number of orientations for performing the orientational average. A measure of the number of dipoles is related to d, the spacing between the dipoles. One wants d to be substantially smaller than the wavelength. The smaller d, the more dipoles are required to fill the volume of the particle. A convenient measure of the spacing in regard to the wavelength is $|m|kd$, where m is the refractive index and $k = 2\pi/\lambda$. Gordon and Du (2001) showed that, for a homogeneous disk with $D = 2.7$ μm, using ~5000 orientations for the orientational average, the error in the backscattering cross section (σ_b) was of the order of 5% for $|m|kd < 0.5$, and decreased rapidly for smaller values of $|m|kd$. In the present work, I always used enough dipoles to keep $|m|kd <$ 0.5 (and often < 0.4) and a number of orientations that would provide approximately the same averaging accuracy as the uniform disk with $D = 2.7$ μm. For the aperiodic pinwheels extensive testing showed that 90,000 orientations were sufficient to perform the averaging.

RESULTS

Although I carried out the computations for pinwheels of three sizes, I will only discuss the first ($D =$ 1.50 μm, $t =$ 0.15 μm, and $n = 5$) in detail here. Figure 3 provides the results of the backscattering cross section computations. Also shown for comparison is the result for a homogeneous disk of the same size (D and t). Note that the homogeneous disk has twice the volume (mass) of the periodic pinwheel ($\varepsilon = 0$) and approximately twice the volume of the aperiodic pinwheels ($\varepsilon > 0$).

Consider first the periodic pinwheels. For these, $s = \lambda/4$ occurs when $t/\lambda = 0.255$. For t/λ larger than this value, the backscattering increases rapidly with decreasing λ and then undergoes a series of maxima and minima with progressively increasing backscattering at each maximum. The backscattering at the maxima is, in magnitude, approximately that at the maxima for the homogeneous disk (twice the volume or mass of the pinwheel). These maxima are the result of interference of the fields scattered by the individual vanes of the pinwheel as they occur in the Rayleigh-Gans approximation as well (although only the first maximum occurs at the same position [Gordon, 2007]). In the case of the smaller aperiodic pinwheel, when $\varepsilon = 0.5$, its backscattering closely follows the periodic pinwheel, with the dispersion of backscattering reaching 20% at the smallest wavelength, while when $\varepsilon = 1.0$ the dispersion is somewhat larger. It is interesting to note that near the position of the first maximum, the aperiodic pinwheel backscatters less than the periodic pinwheel, and the deviation between the two increases with increasing ε. This behavior would be expected under the hypothesis that the maxima in the periodic case results from constructive interference of light interacting with the individual vanes of the pinwheel – when the spacing and angular size of the vanes becomes random the constructive interference is reduced.

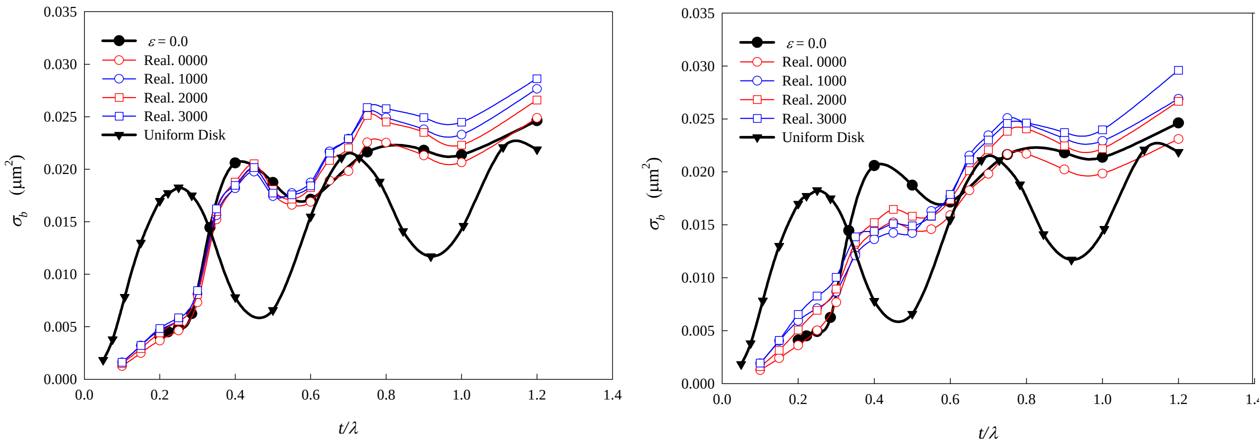


Figure 3: The backscattering cross section of four realizations of the aperiodic pinwheels shown in Figure 1 (D = 1.5 μm) compared with that for a periodic pinwheel and for a homogeneous disk of the same size as a function of the thickness divided by the wavelength.   The left panel is for $\varepsilon = 0.5$ and the right panel is for $\varepsilon = 1.0$. The periodic pinwheel shows increasing (and oscillatory) backscattering with decreasing wavelength. The individual realizations of aperiodic pinwheels all roughly follow their periodic counterpart, but with dispersion that increases with increasing ε.

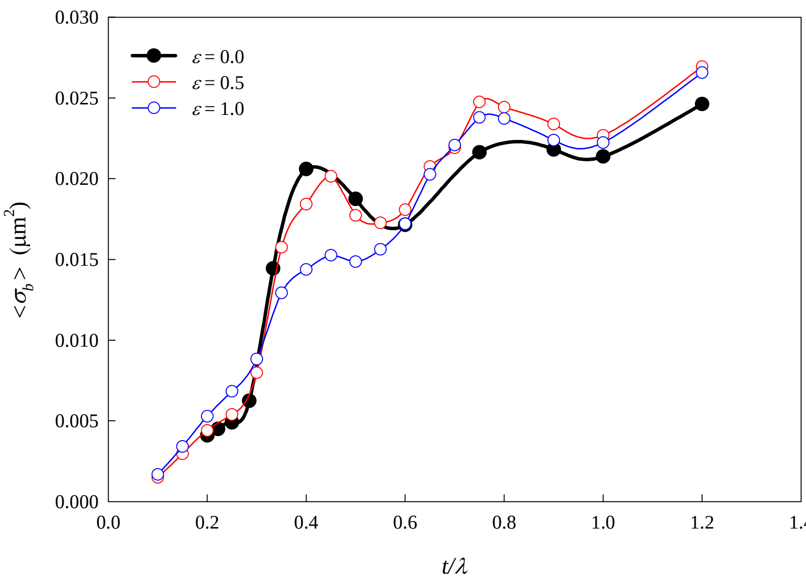


Figure 4: The backscattering cross section $\langle \sigma_b \rangle$ of an equal-number mixture of the four realizations of the aperiodic pinwheels compared with that for a periodic pinwheel ($\varepsilon = 0$). This shows that the $\varepsilon = 0.5$ cases are close to the periodic pinwheel, but for $\varepsilon = 1.0$, the deviation is considerable, especially near the first maximum for $\varepsilon = 0$.

It is important to understand that real biological particles (e.g., *E huxleyi* coccoliths) would display similar dispersions in backscattering. In fact, if pinwheels were to represent real biological particles, samples would be expected to consist of a number of realizations of their aperiodicity. In this regard, the average σ_b (denoted by $\langle\sigma_b\rangle$) is more important than that for any given realization. Figure 4 compares the $\langle\sigma_b\rangle$ for the four realizations of the aperiodicity examined here with the associated periodic pinwheel. It clearly shows that the main difference between $\langle\sigma_b\rangle$ for the small periodic and aperiodic pinwheels (left panel) occurs near the maxima in the backscattering, and that near the first maximum (but not the second) the difference increases as deviation from periodicity increases (i.e., as ε increases).

The computations for the two other examples of aperiodic pinwheels (D = 1.5 μm, t = 0.05 μm, n = 5, and D = 2.75 μm, t = 0.05 μm, n = 6) revealed that as D/t becomes larger, the dispersion among realizations decreases somewhat, and $\langle\sigma_b\rangle$ becomes very close to that of the associated periodic pinwheel.

IMPACT/APPLICATIONS

I examined the deviation in the angular spacing of the "spokes" in the distal shield of the individual coccoliths provided in Fig. 2 of Gordon (2006). For this particular coccolith, $\sigma_{\Delta\alpha}/\Delta\alpha$ ~ 0.27, and there were 40 open angular sectors. This coccolith shield is similar in size and shape to the larger (2.75 μm) pinwheel (n = 6, 32 open sectors) I examined. The computations for the that pinwheel (not shown) suggested that, for the purpose of computing backscattering, the periodic pinwheel is a good approximation to aperiodic pinwheel as long as $\sigma_{\Delta\alpha}/\Delta\alpha \le 0.4$ ($\varepsilon \le 1$). This suggests that replacing the aperiodic fine structure of the distal shield of *E. huxleyi* coccoliths with a strictly periodic fine structure will not degrade the modeling of their backscattering, especially for natural samples containing large numbers of coccoliths.

REFERENCES

Draine, B.T., The discrete-dipole approximation and its application to interstellar graphite grains. *Astrophys. J.* **333**: 848–872, 1988.

Draine, B.T. and P. Flatau, "Discrete-dipole approximation for scattering calculations," J. *Opt. Soc. Am. A* **ll,** 1491–1499, 1994.

Gordon, H.R. and Tao Du, Light scattering by nonspherical particles: application to coccoliths detached from *Emiliania huxleyi*, *Limnology and Oceanography*, **46**, 1438–1454, 2001.

Gordon, H.R., Backscattering of light from disk-like particles: is fine-scale structure or gross morphology more important?, *Applied Optics*, **45**(27), 7166–7173, 2006.

Gordon, H.R., Rayleigh-Gans scattering approximation: surprisingly useful for understanding backscattering from disk-like particles. *Optics Express*, **15**, 5572-5588, 2007.

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